Predicting Transport Integrals with Machine Learning

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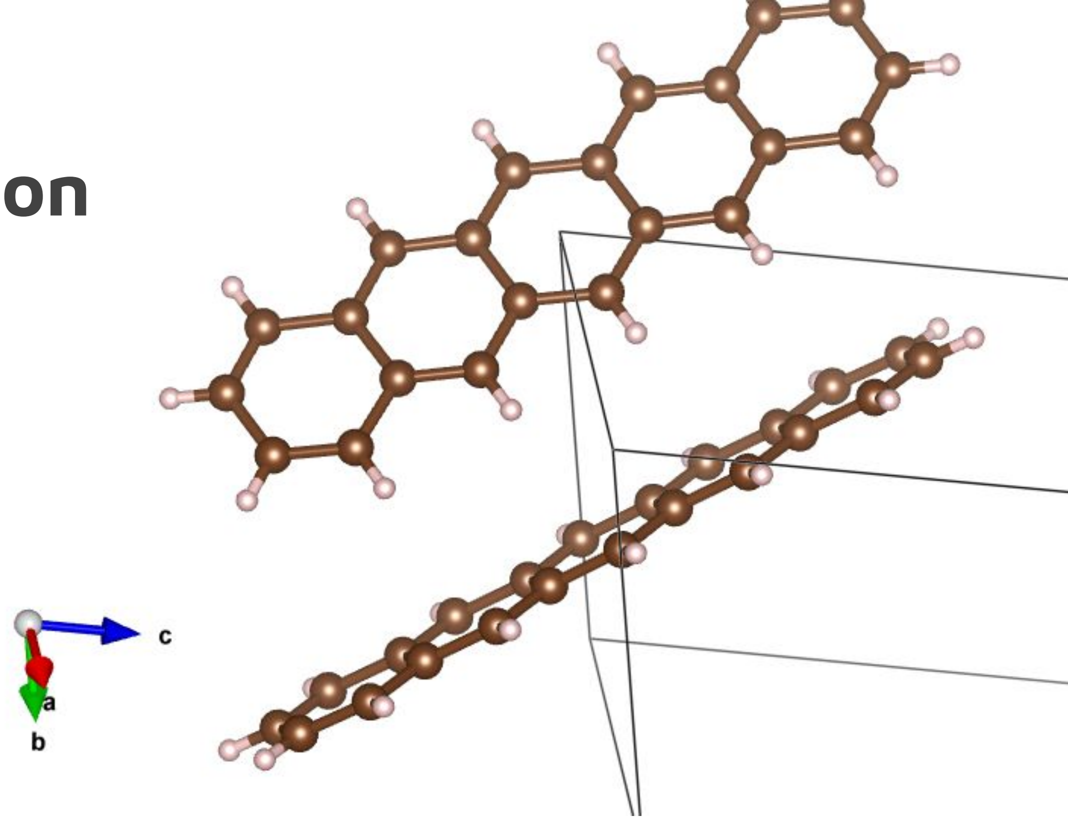
Quick Recap

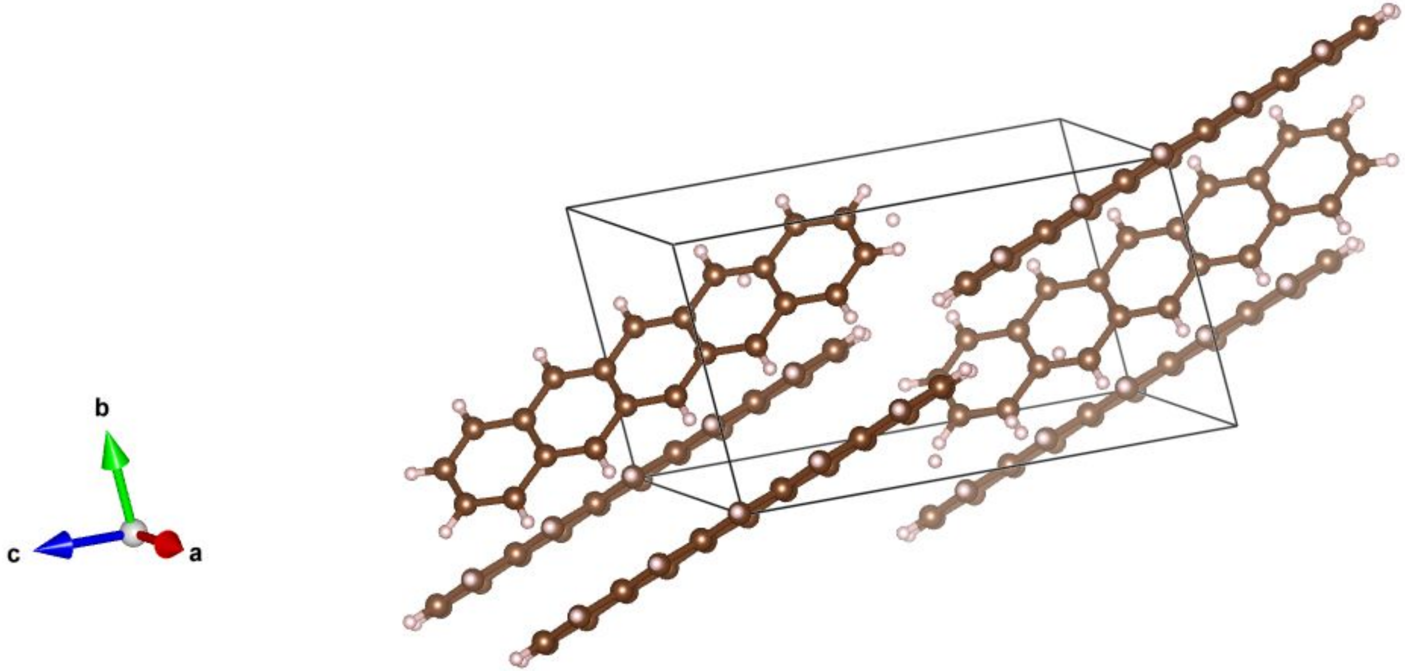
Given Information

Pic file with 900 features and 10,000 example



Goal

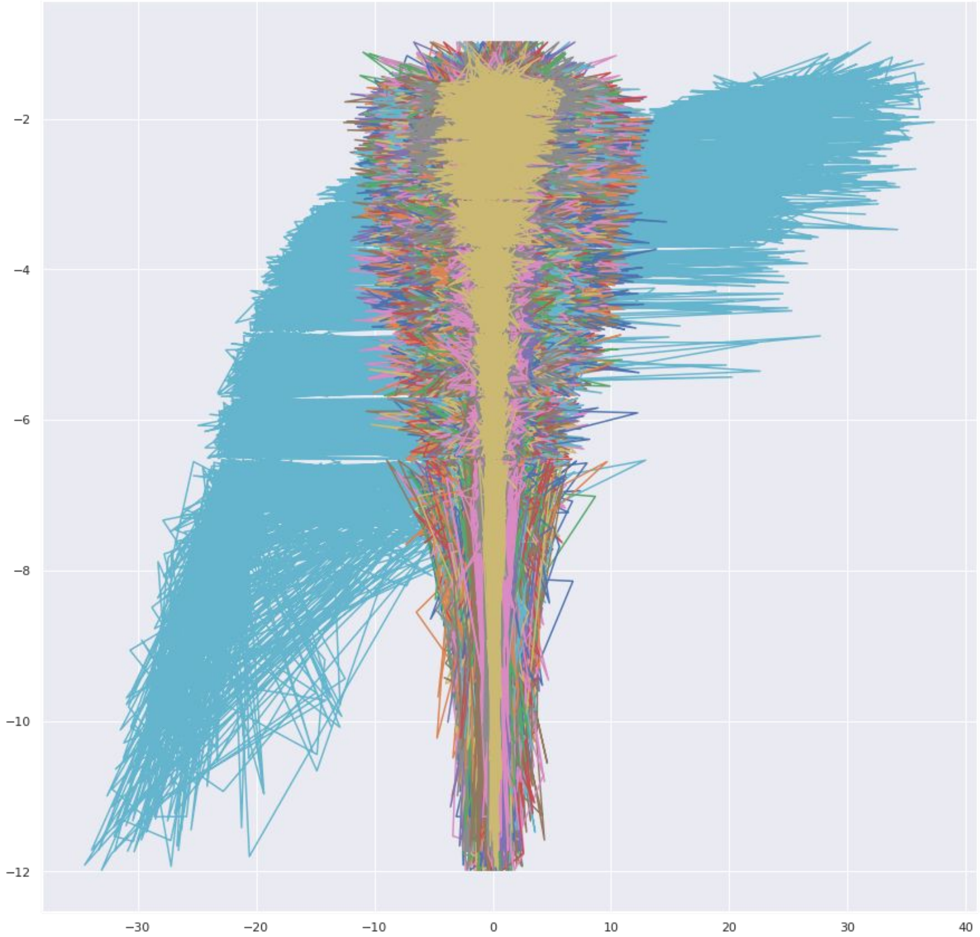
Predict the Transport integral give 900 distances between two 30-atom monomers



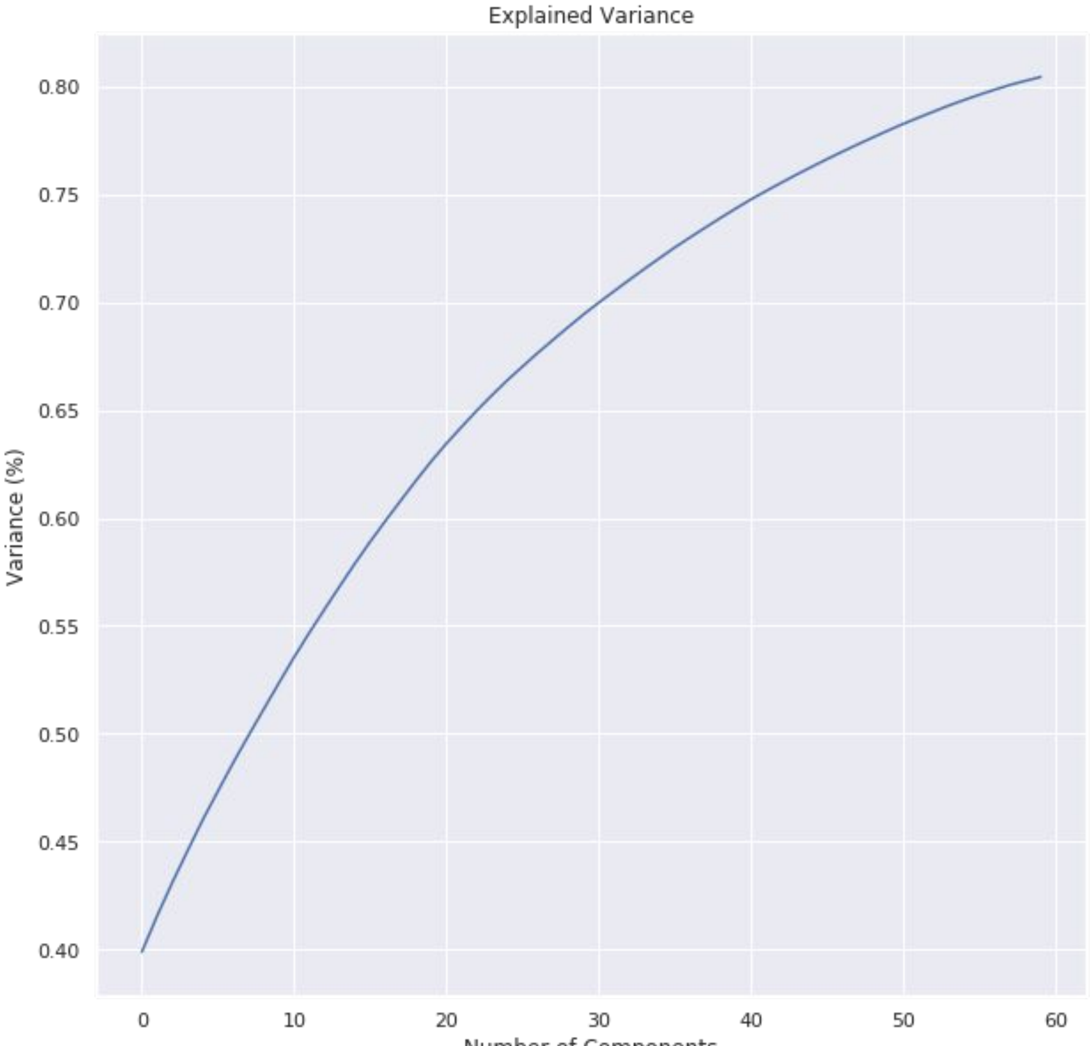
Preprocessing

Dealing with 900 features

Principal Component Analysis



PCA Cont.



Explained Variance
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
Variance (%)
0
10
20
30
40
50
60
Number of Components

Regularization for Model Fitting

Add an extra cost to the loss function to prevent overfitting

L1 vs. L2

Regularization for Model Fitting

L1: Lasso Regression

- Loss function = sum of absolute values of errors
- (**L**east **A**bsolute **S**hrinkage and **S**election **O**perator)
- Tends to push weights to zero

$$\sum_{i=1}^{n}(Y_i - \sum_{j=1}^{p} X_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

L2: Ridge Regression

- Loss function = sum of squared errors

$$J(\theta) = \frac{1}{2m}\left[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \boxed{\lambda \sum_{j=1}^{n} \theta_j^2}\right]$$

$$\min_{\theta} J(\theta)$$

Lasso shrinks the less important features' coefficients (even removing them altogether), making it better for feature selection with large number of features

Regression Models

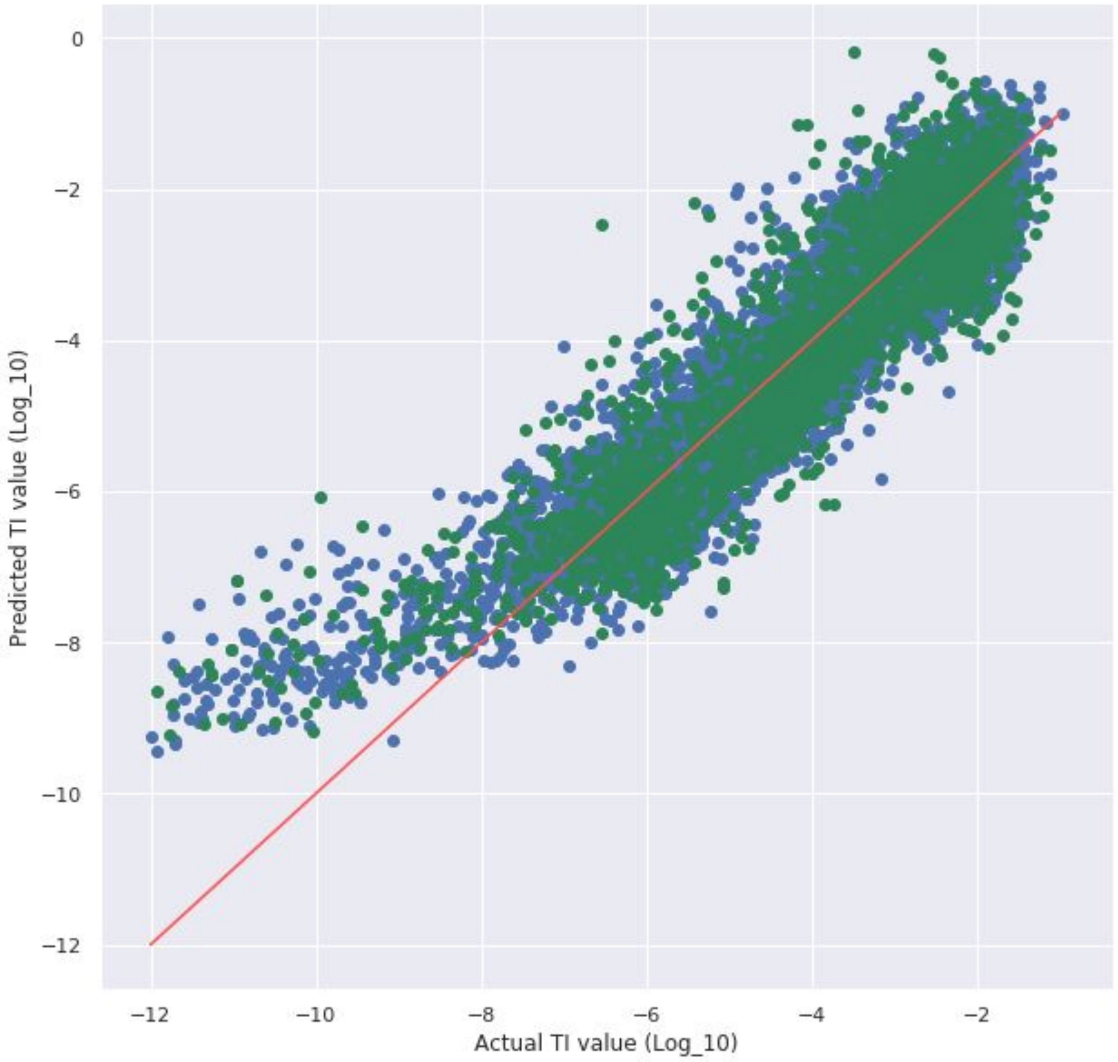
Linear Regression

With PCA applied and k-fold cross validation:

Mean_squared_error (average):
1.002949261587887
standard_deviation:
1.187689627016626

(RMSE: 1.0014735)

Training Data: Y vs. Y_prediction
Test Data: Y vs. Y_prediction
(Linear with slope 1 => perfect match)



Sanity check: How is PCA doing?

Without PCA

```
RMSE:
0.795003 (no k-fold)

mean_squard_error:
1.002949261587887

standard_deviation:
1.187689627016626
```

With PCA

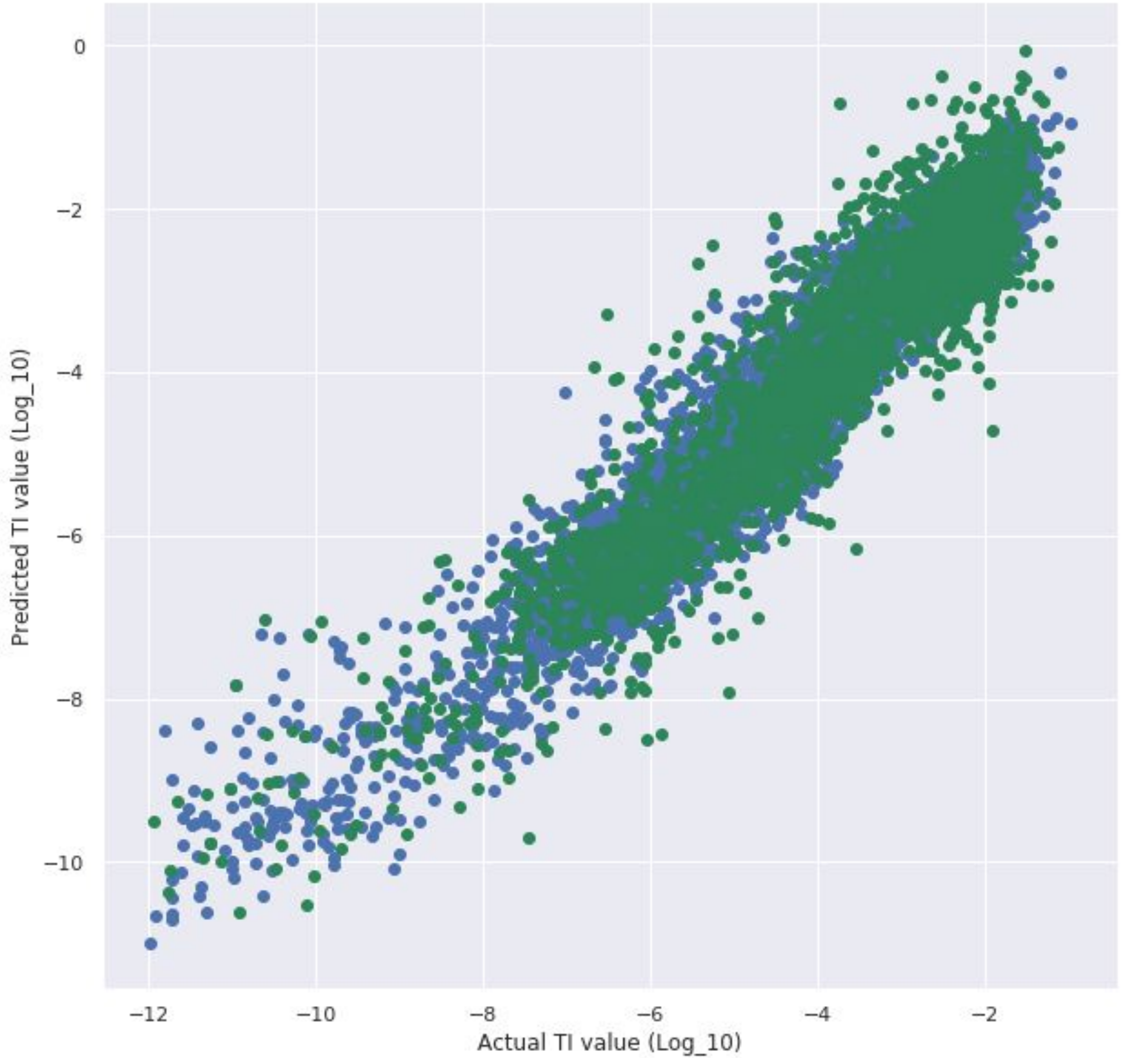
```
RMSE:
1.129056 (no k-fold)

mean_squard_error:
1.002949261587887

standard_deviation:
1.187689627016626
```

Polynomial Regression

Mean_squared_error (average):
1.774617823490909

standard_deviation:
2.4438984231990983

(RMSE: 1.3321478234381157)



Training Data: Y vs. Y_prediction
Test Data: Y vs. Y_prediction

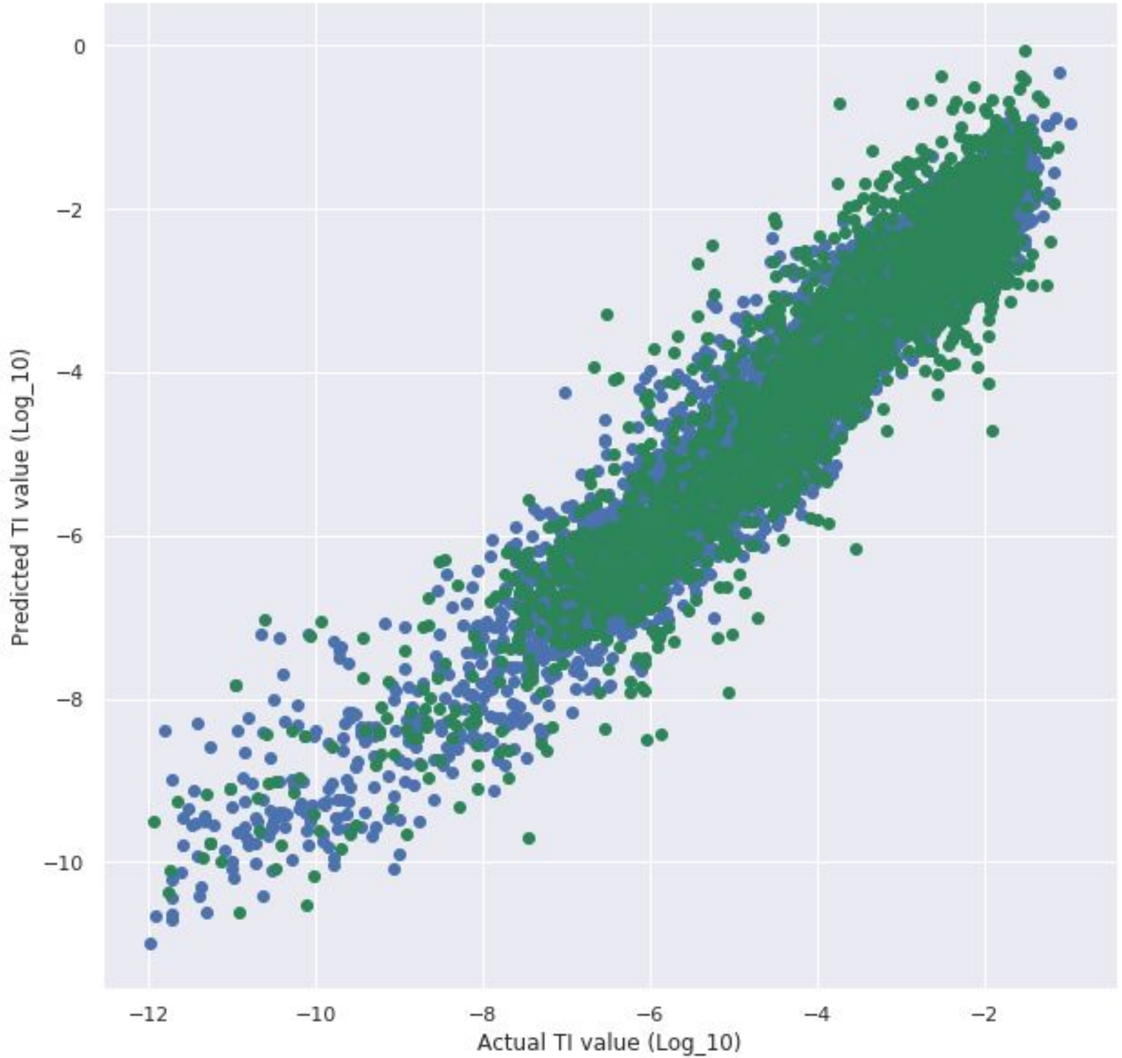
Polynomial Regression

Mean_squared_error (average):

1.774617823490909

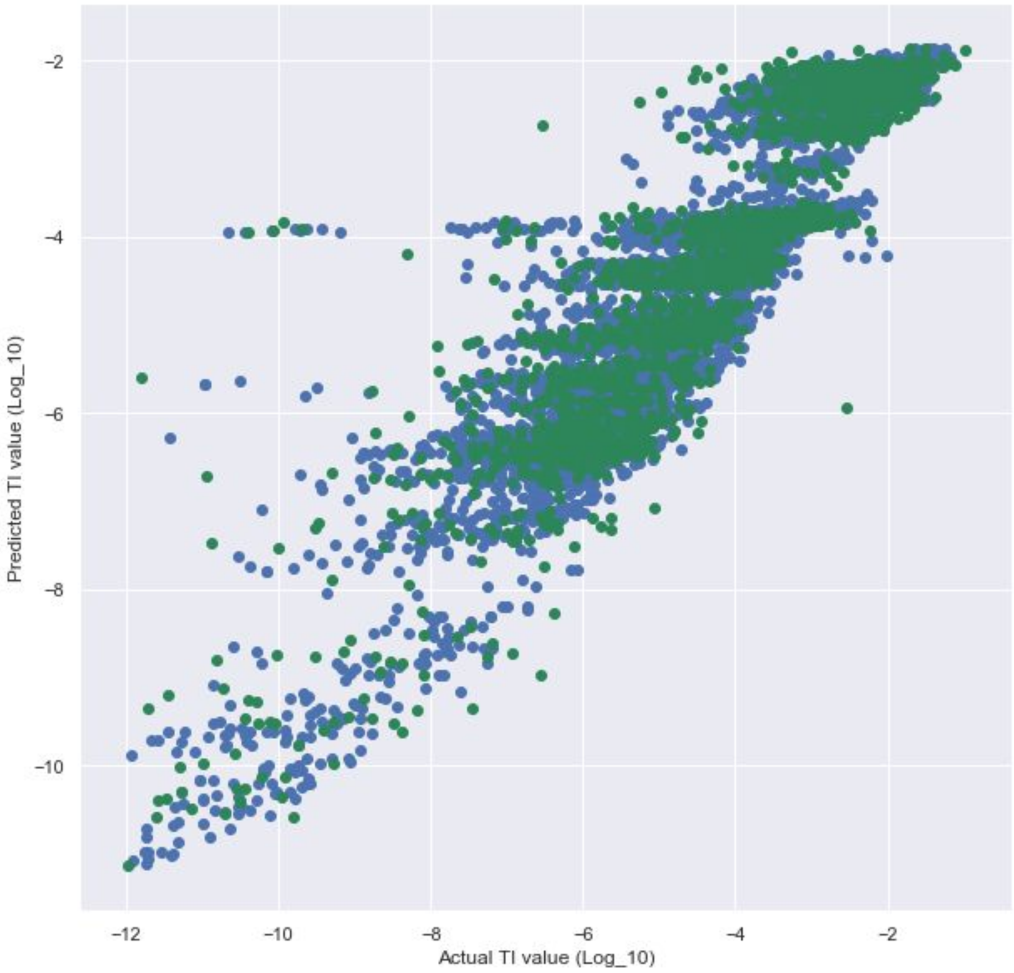
mean_squared_errors: [8.92539671
1.24277882 0.53544367 0.97998094
1.85069762 1.98805718 0.88201865
0.455358   0.37556103 0.51088562]

Training Data: Y vs. Y_prediction
Test Data: Y vs. Y_prediction



Random Forest Regressor

- best parameters are max_depth of 6 and n_estimators of 1000
- RMSE: 0.699682

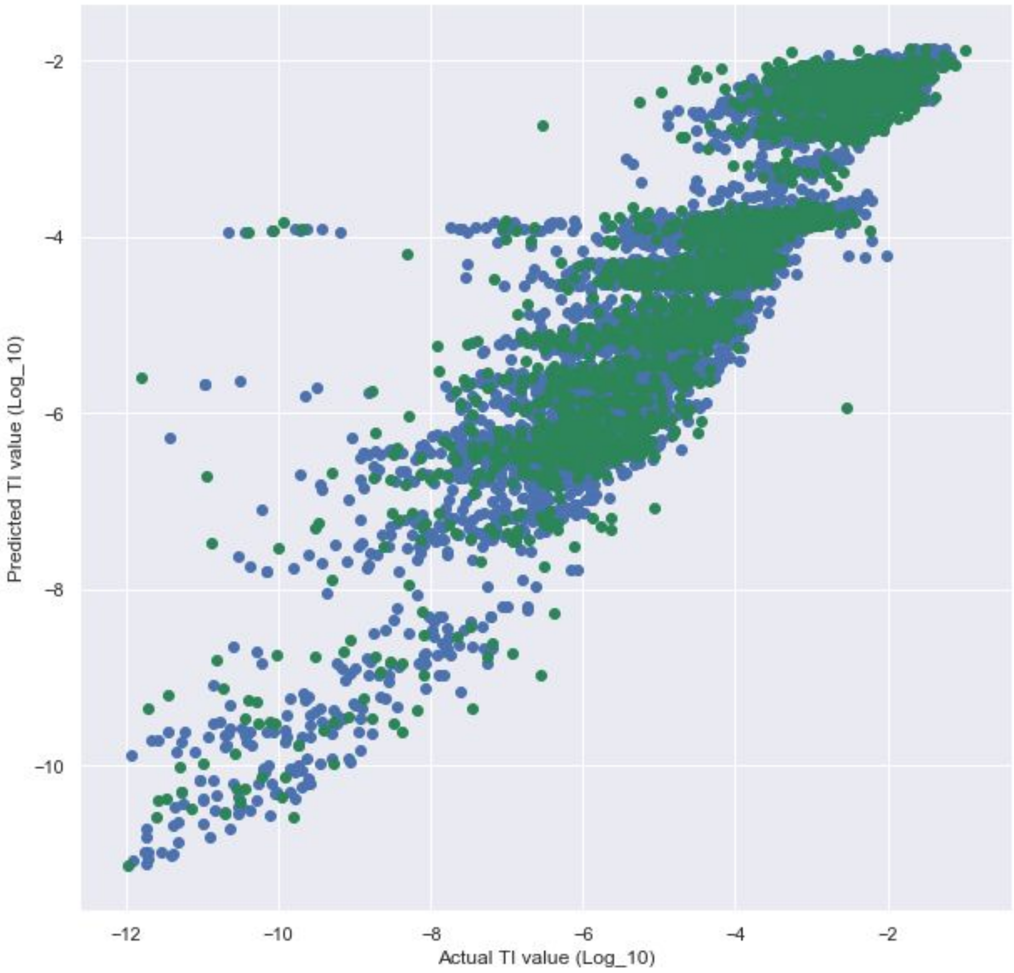


Random Forest Regressor

[6.35710053 0.71129973
0.79274011 0.58765779
0.48054221 0.75907597
0.38439998 0.17103299
0.18910843 0.59895555]

mean_squared_error:
1.1031913291487907

standard_deviation:
1.763541449709036



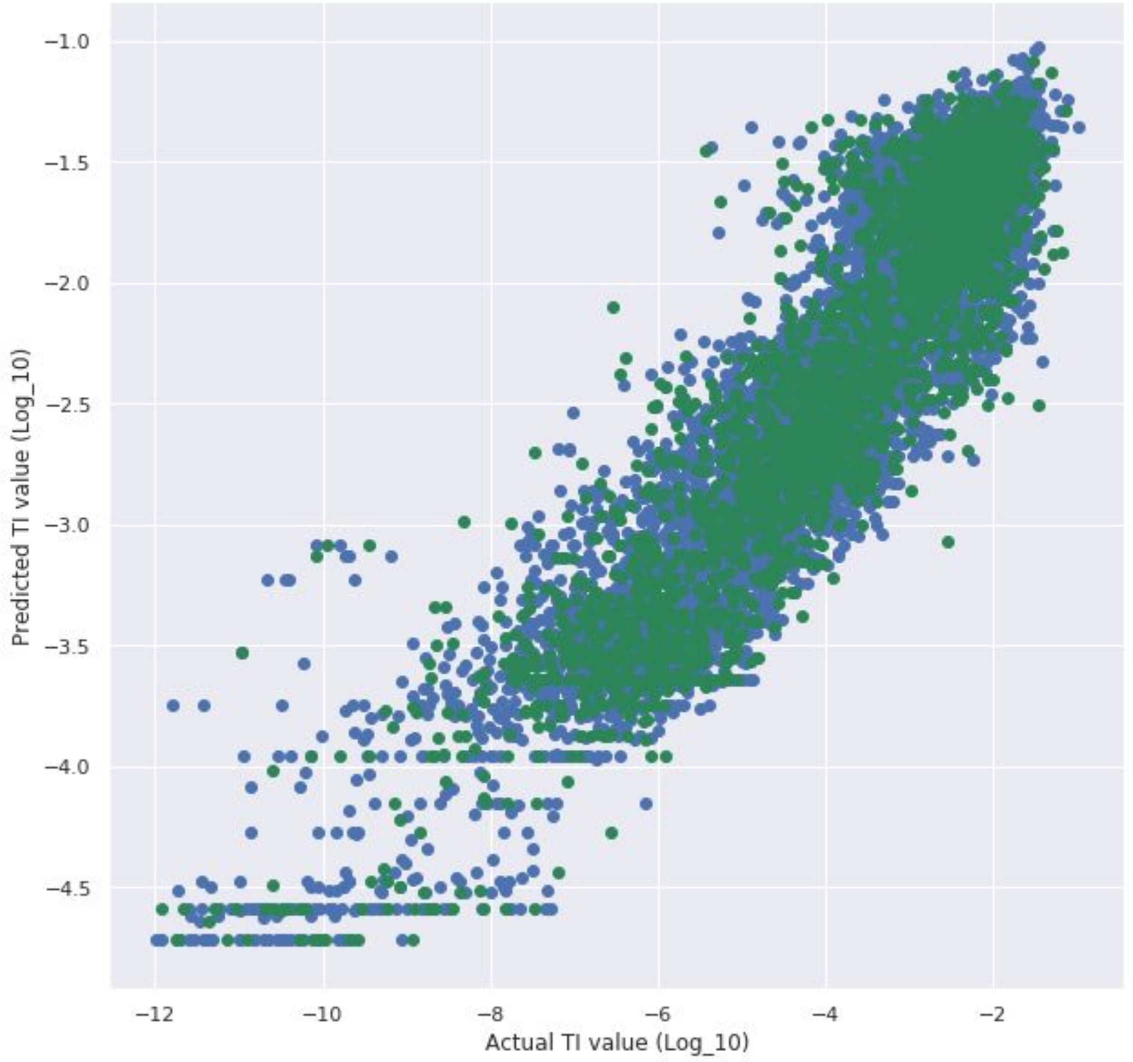
Training Data: Y vs. Y_prediction
Test Data: Y vs. Y_prediction

XGBoost Regressor

RMSE: 1.999990

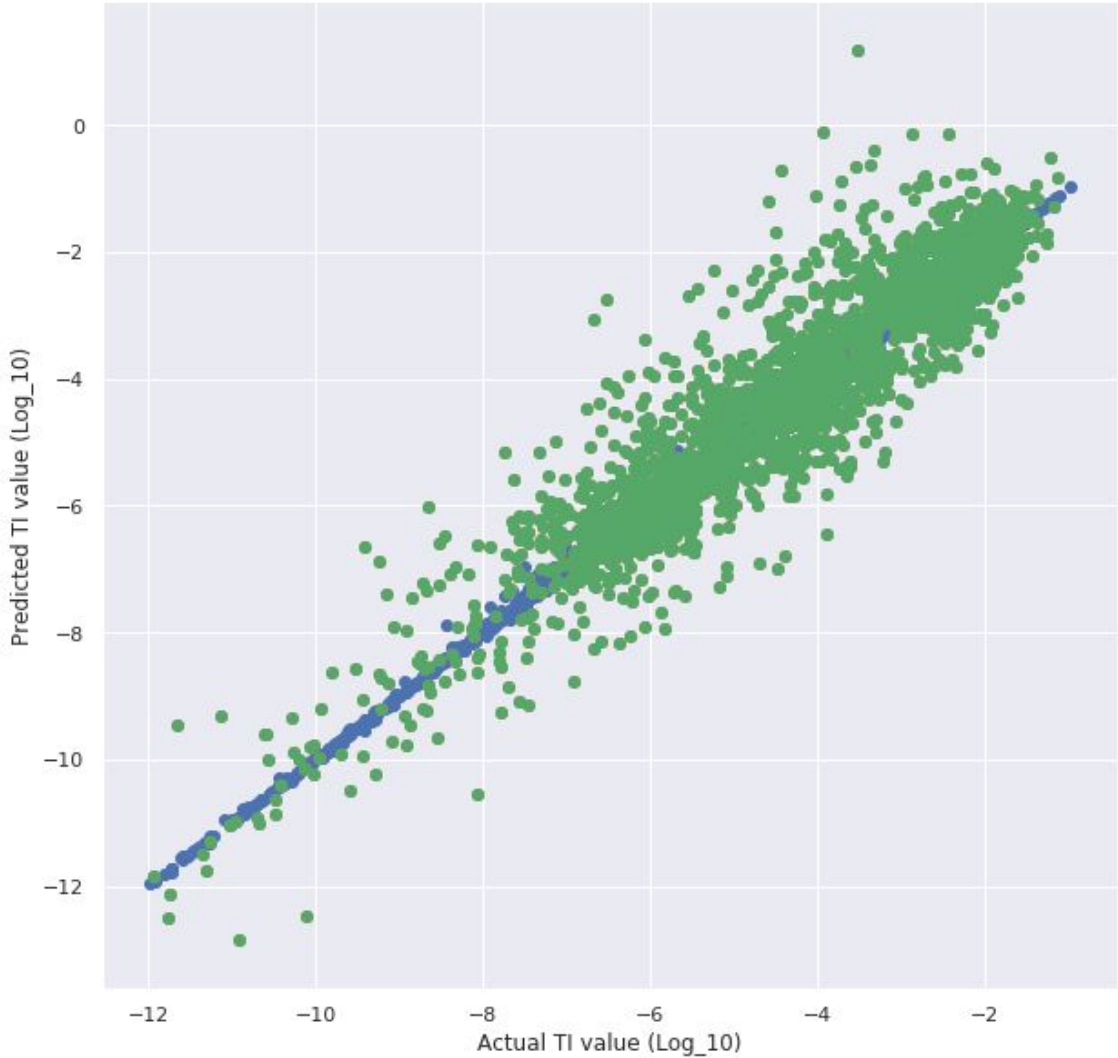
```
xgboost =
xgb.XGBRegressor(objective
='reg:squarederror',
colsample_bytree = 0.3,
learning_rate = 0.1, max_depth =
5, alpha = 10, n_estimators =10)
```

Training Data: Y vs. Y_prediction
Test Data: Y vs. Y_prediction



Kernel Ridge

RMSE of 0.799

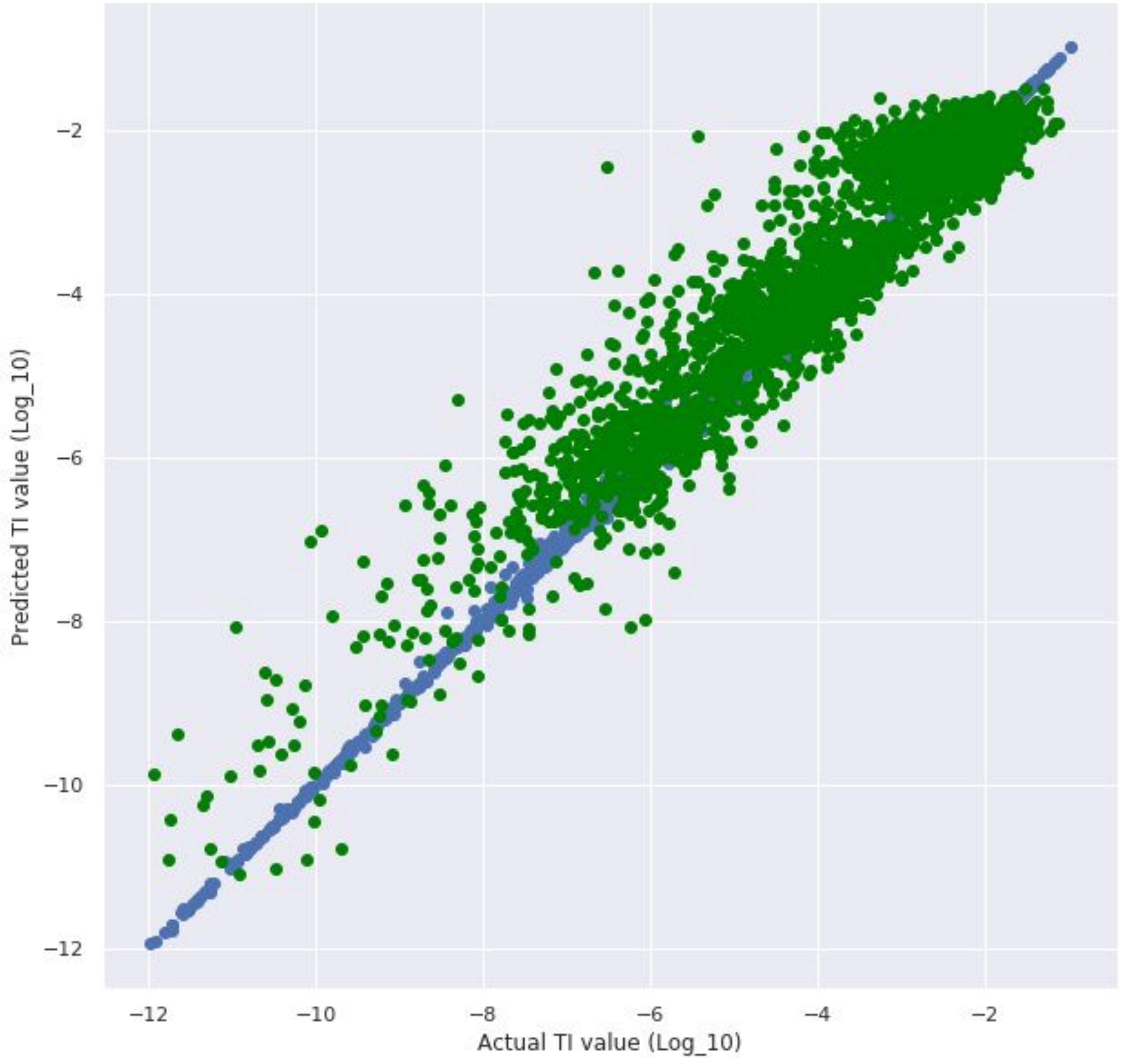


Training Data: Y vs. Y_prediction
Test Data: Y vs. Y_prediction

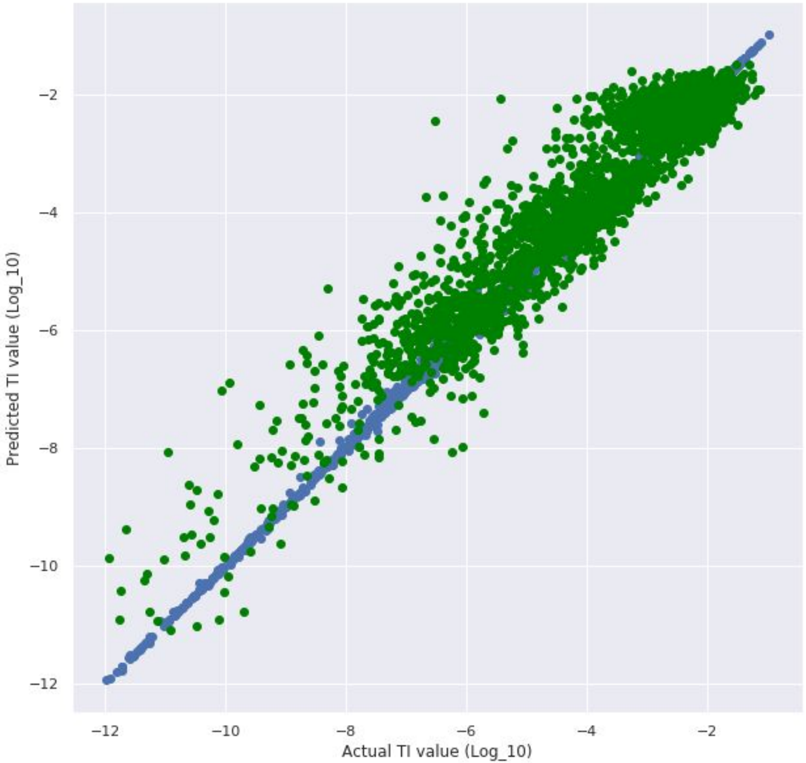
Keras Neural Network

RMSE: 0.645438

Training Data: Y vs. Y_prediction
Test Data: Y vs. Y_prediction

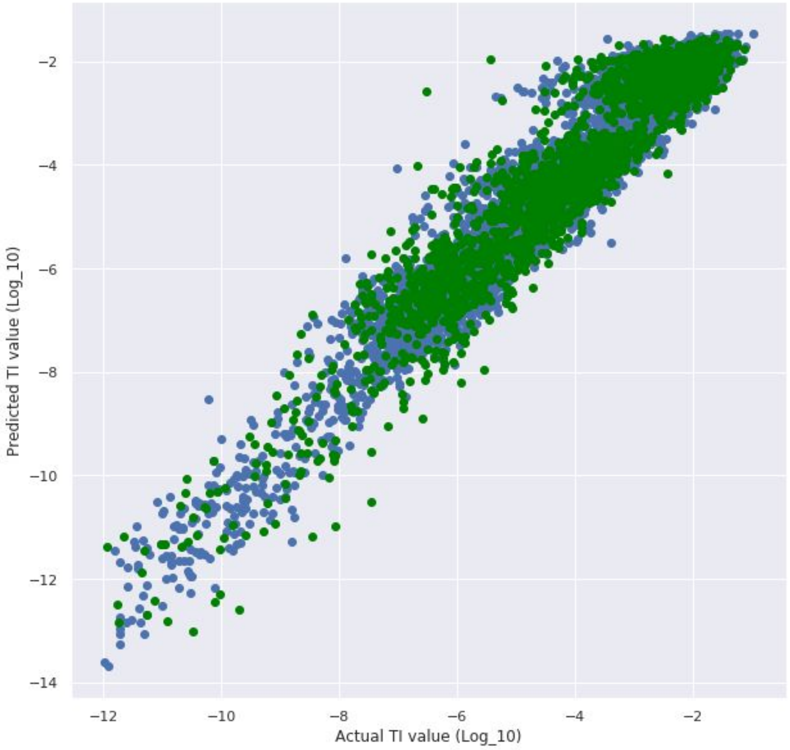


Correcting Keras Overfitting



Loss = mean_absolute_error

RMSE: 0.640988



Loss = mean_squared_error

RMSE: 0.575086

Final Predictions

Keras

```
#fit keras
neuraln = Sequential()
neuraln.add(Dense(128, input_dim=60, activation='relu'))
neuraln.add(Dense(256, kernel_initializer='normal',activation='relu'))
neuraln.add(Dense(256, kernel_initializer='normal',activation='relu'))
neuraln.add(Dense(256, kernel_initializer='normal',activation='relu'))
neuraln.add(Dense(1, kernel_initializer='normal', activation='linear'))
neuraln.compile(loss='mean_absolute_error', optimizer='adam', metrics=['mean_absolute_error'])
neuraln.fit(x_pca, y, epochs=100, batch_size=10)
y_pred = neuraln.predict(x_test_pca)
y_pred = 10 ** y_pred #undo the y = np.log10(TI_df) used by the training
```